10,11-Dihydro-5H-dibenz(b,f)azepin-5-amine
7458-07-3 | DTXSID00225559

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 3.22e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.68e-01

Confidence level: 4.40e-01

Nearest Neighbors from the Training Set

Image not found
Phenanthrene
Measured: 5.60e-05
Predicted: 2.07e-05

Image not found
Phenanthridine
Measured: 2.18e-04
Predicted: 1.01e-04

Image not found
Triphenylene
Measured: 2.08e-05
Predicted: 1.87e-08

Image not found
2,3-Benzofluorene
Measured: 1.35e-04
Predicted: 2.22e-07

Image not found
Fluorene
Measured: 7.50e-07
Predicted: 9.71e-04